

Heptafluorobutyric acid
375-22-4 | DTXSID4059916

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.47

Global applicability domain: Outside

Local applicability domain index: 2.84e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

Image not found

Sodium 3-nitrobenzenesulfonate

Measured: 5.01

Predicted: 5.24

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4-Hydroxy-1-naphthalenesulfonic acid monosodium salt

Measured: 12.9

Predicted: 6.33

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Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

Measured: 3.02

Predicted: 5.14

Image not found

2-Amino-5-methylbenzenesulfonic acid

Measured: 3.98

Predicted: 6.29

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2-Amino-1-naphthalenesulfonic acid

Measured: 6.03

Predicted: 6.40